Haldane-like Chern insulators in buckled lattices with in-plane magnetic fields

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Chern insulators, first proposed by Haldane over 20 years ago, has not been observed experimentally. While there is some expectation that topological insulators with broken time reversal symmetry may realise the phase, the mechanism – spin orbit interaction together with magnetic exchange – has a completely different origin to Haldane's staggered magnetic field. I show that buckled lattices with in-plane magnetic fields are a promising route to realising Haldane-like models. As a concrete example, I consider silicene, a honeycomb lattice with out-of-plane sublattice anisotropy, in an in-plane magnetic field, and show that it is a Chern insulator insulator, even at negligibly small magnetic fields, which is analogous to Haldane's original model, though bears some interesting differences as well.

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F.D.M. Haldane's 1988 paper, 'Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"' [1], was a paradigm shifting work which is undoubtedly a precursor to the field of topological insulators [2–4]. In fact, topological insulators in an external field, or in the presence of ferromagnetic exchange coupling, are thought to be Chern, or quantum anomalous Hall (QAH) insulators [5], of which Haldane's model is the seminal example. An ultracold gas implementation of Haldane's model was recently proposed, which utilised laser induced pseudomagnetic fields to produce a staggered flux [6, 7].

Both Haldane's original model, and the more recent topological insulators, are based on Dirac cone physics. The most straightforward statement of this is in terms of linear Dirac equations: two adjoining systems with massive (gapped) Dirac cones, with Hamiltonians $H_\pm = (k_x, k_y, \pm m)\cdot\vec{\sigma}$, supports gapless edge states at their interface due to the change in sign of the mass between the two systems. In real systems, this amounts to having an effective mass term which is oppositely signed to that of the vacuum. At the interface between the system containing the cone, and the vacuum then, there is a point at which $m \to 0$, and the band gap closes. The quantum anomalous Hall phase is that where there is a single (Mod(2)) zero energy species on the edge of a system. The quantum spin Hall phase is that where there are two (Mod(2)) counter-propagating edge states, as there must be if time reversal symmetry is not broken.

In this Letter, I show that Haldane-like models can be constructed, using the same mechanism, of a staggered magnetic flux, as in Haldane's original proposal, by employing an in-plane magnetic field incident on a buckled two dimensional system. Using a concrete example, I construct a Hamiltonian which realises the same chiral states as in the original model, and yet does not have the same chiral structure of flux accumulation. The orientation of the incident field can also induce phase transitions between the QAH and ordinary insulating states.

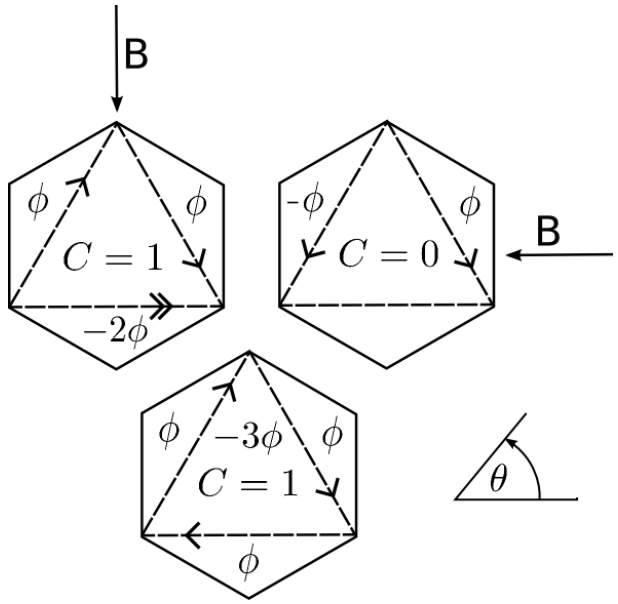

FIG. 1: Hexagonal unit cells with zero net magnetic flux. The upper two unit cells are a buckled honeycomb lattice (e.g. silicene) in an in-plane magnetic field. Due to the buckled lattice structure, closed loops of nearest and next-nearest neighbor bonds have either a positive or negative flux passing through them. In the lower pane is shown Haldane's unit cell [1], where the flux (from a spatially inhomogeneous perpendicular magnetic field) through the outer three loops are compensated by an opposing flux through the centre. In each case, the direction of positive flux accumulation is indicated by the arrows along the bonds. Note that I have only shown the bonds along a single sublattice for clarity.

Silicene is a two dimensional honeycomb lattice, where the two sites in the unit cell are offset from each other, in the out-of-plane direction. I define the plane parallel to the lattice, $z = 0$, such that one triangular sublattice is at $z = l$, and the other at $z = -l$. The silicene Hamiltonian in an in-plane magnetic field and an out-of-plane electric field then, is [9]:

$$H = t\sum_{\langle i,j\rangle,} c_i^\dagger c_j + \sum_{\langle\langle i,j\rangle\rangle,} t'_{ij} c_i^\dagger c_j + \Delta\sum_{i,} \nu(i) c_i^\dagger c_i, \quad (1)$$

where t is the nearest neighbor hopping integral, $t'_{ij} = t'\exp(i\frac{e}{\hbar}\int_i^j \vec{A}\cdot d\vec{l})$ is the Peierl's substitution modified next nearest neighbor hopping, $\Delta = lE_z$ is the electric field multiplied by the out-of-plane buckling $l = 0.23\mathring{A}$. The out-of-plane field is not necessary to observe the QAH effect, but allows us to make contact with Haldane's work, and when including spin effects, becomes important. I have chosen a gauge such that the flux is accounted for on next nearest neighbor bonds. We are free to choose any consistent gauge such that the total phase accumulated over closed loops encircling regions of some flux is always commensurate with that flux. Due to the definition that $z = 0$ defines the lattice plane such that the two sublattices are at $z = \pm l$, the particular gauge choice in which nearest neighbor flux accumulation vanishes, is the Landau gauge, $\vec{A} = Bz(\sin\theta, -\cos\theta, 0)$, where θ is the angle of the field relative to the horizontal direction in Fig.[1]. The Hamiltonian, in momentum space, becomes

$$H_{\vec{k}} = \vec{c}_{\vec{k}}^{\,\dagger}\big(d_0(\vec{k})\sigma_0 + \vec{d}(\vec{k})\cdot\vec{\sigma}\big)\vec{c}_{\vec{k}}, \quad (2)$$

where $\vec{c}_{\vec{k}}^{\,\dagger} = (c^\dagger_{A,\vec{k}}, c^\dagger_{B,\vec{k}})$, and in which $d_0(\vec{k}) = \cos(\phi/\phi_0)\sum_i^3 2t'\cos(\vec{k}\cdot\hat{\delta}'_i)$, where $\phi_0 = h/2e$, and ϕ/ϕ_0 is the integrated gauge field over the bond using the Landau gauge, which gives the total flux through the loop with one next nearest neighbor and two nearest neighbor bonds ($\phi = Bla$, with a the lattice constant), as indicated in Fig.[1]. δ'_i are three out of six of the next nearest neighbor vectors defined by $\delta'_n = R(2\pi n/3)(1,0)$, where $R(\theta)$ rotates the vector by θ, and

$$\vec{d}(\vec{k}) = \sum_i^3 \big(\mathrm{Re}(te^{i\vec{k}\cdot\delta_i}), \mathrm{Im}(te^{i\vec{k}\cdot\delta_i}), \Delta - \sin(\phi/\phi_0)2t'\sin(\vec{k}\cdot\hat{\delta}'_i)\big), \quad (3)$$

where δ_i are the three nearest neighbor vectors defined by $\delta_n = R(2\pi n/3)(0, -1/\sqrt{3})$.

This particular choice of gauge makes concrete contact with Haldane's original choice, as well as being intuitively and computationally convenient. The system, together with the inclusion of flux along the bonds, and the comparison with Haldane's model, are all shown in Fig.[1]. The chirality, noted by Haldane in his model, is the clockwise accumulation of positive flux over next nearest neighbor hops. The clockwise accumulation of positive flux is clear in the lower panel in Fig.[1]. This chirality is absent in the buckled lattices (i.e. the upper two unit cells shown in Fig.[1]), where hopping over the equivalent loop leads to zero phase accumulation. However, a triangular loop comprising one next nearest neighbor and two nearest neighbor hops acquires a non-zero positive phase. For the upper left panel, there are two loops which acquire a negative phase on clockwise hopping, and one which acquires a negative phase. There is, therefore, a net chirality. In the upper right however, the lower triangular plaquette envelopes no magnetic flux, and thus there are just two oppositely oriented chiral loops, and thus no net chirality.

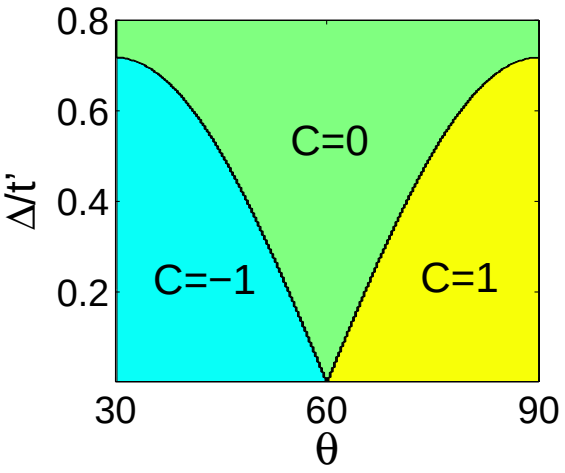

FIG. 2: Phase diagram for spinless silicene in an in-plane magnetic field (such that $\phi/\phi_0 = \pi/2$), where $\Delta = El$. Here θ is the angle of the in-plane field. The angles $\pi/6$ and $\pi/2$ correspond to the upper left orientation of the field in Fig.[1], whereas the angle $\pi/3$ corresponds to the upper right.

The Hamiltonian Eq. [2] describes a graphene-like system with two low energy Dirac cones at the two inequivalent K points, $K_\pm = (\pm 4\pi/3, 0)$. At $\Delta, B = 0$, the system is exactly the graphene system, where the low energy Dirac cones are massless. Δ and B then introduce separate mass terms. The Δ mass term is due to the on-site energy imbalance between the two sublattices due to the electric field Stark effect. The magnitude of this gap is $2El$. The second, which I call the 'flux gap', is the sublattice anisotropy due to the orbital effect of the magnetic field, and its magnitude is

$$\Delta_\phi = \sqrt{3}t'|2\sin(\phi/2\phi_0) - \sin(\phi/\phi_0)|\sin(3\theta). \quad (4)$$

This gap goes as $(\phi/\phi_0)^3$ for small fields, and so may be tiny for realistic laboratory fields. Later, I will discuss ways in which this number can be improved by several orders of magnitude in the lab.

Since the flux gap is $\propto \sin(\vec{k})$ (i.e. the z-component of Eq. [3]), it has opposite sign in the two valleys (the two Dirac, or K, points). Therefore, Δ and Δ_ϕ add, or compete, in the two valleys, as is clear from Fig.[4], such that the gap in the two valleys, are $\Delta_{K_\pm} = \Delta \pm \Delta_\phi$.

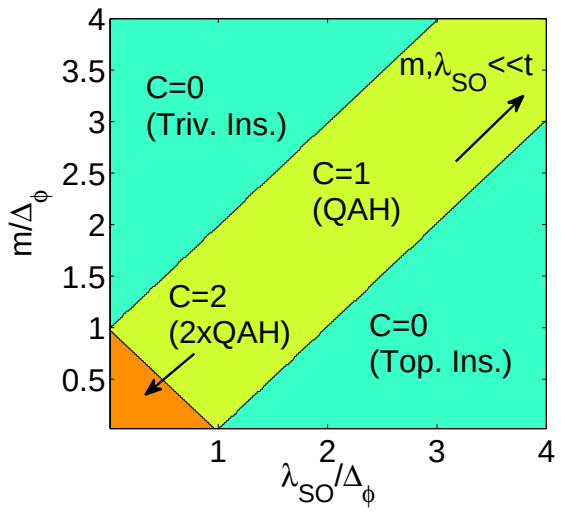

FIG. 3: Phase diagram including both spins in silicene. For small spin orbit coupling and small electric field, we obtain two co-propagating chiral bands. This is equivalent to a $\nu = 2$ quantum Hall effect, or equivalently, a doubled Chern insulator. For an electric field gap larger than the flux gap, the system is a trivial insulator, as also noted in Fig.[2]. For small electric field gap, but comparatively large spin orbit coupling, silicene is a Kane-Mele topological insulator [2]. However, when $\lambda_{SO}+m > \Delta_\phi$, but $|\lambda_{SO}-m| < \Delta_\phi$, silicene is a Chern insulator with a single chiral band, equivalent to a $\nu = 1$ quantum Hall effect. In principle, the diagonal $C = 1$ section of the phase diagram continues indefinitely, so long as the energy scales $m \sim \lambda_{SO} \ll t$, such that the K points are not mixed by these terms.

The quantum anomalous Hall (QAH) phase is characterised by a Chern number of 1 (Mod(2)), where the Chern number is the integral of the Berry curvature over the Brillouin zone [10]. For our Hamiltonian Eq. [1], it takes the particularly simple form [3, 12]

$$C = \frac{1}{4\pi}\int_{BZ} d\mathbf{k}\hat{d}\cdot\frac{\partial\hat{d}}{\partial k_x}\times\frac{\partial\hat{d}}{\partial k_y} \overset{K_\pm}{=} \frac{\mathrm{sgn}(\Delta_\pm)}{2}, \qquad (5)$$

where the second equality is the result for the Hamiltonian Eq. [1] expanded to first order in $\vec{k}$ near the $K_\pm$ points. From the second equality, we suspect, and it is confirmed by taking the integral Eq. [5] over the entire Brillouin zone, that the Chern number is

$$C_n = \begin{cases} 1 & \Delta_\phi > \Delta \\ 0 & \Delta_\phi < \Delta. \end{cases} \qquad (6)$$

In Fig.[2] is shown the Chern number phase diagram of Hamiltonian Eq. [1], as a function of in-plane field orientation θ, where $\theta = 0$ corresponds to a field along the zig-zag direction, as shown in the upper right portion of Fig.[1]. At $\Delta = 0$, the Chern number is ± 1 for *almost* the entire spectrum of field orientations. This can be understood by considering Fig.[1]. For all θ except $\pi n/3$, there is a positive flux passing through either one or two plaquettes in the unit cell, and a negative flux passing through two or one, such that the total flux is always zero. The positive fluxes instigate cyclotron motion around the triangular plaquettes in one direction, while the negative flux instigates cyclotron motion in the opposite direction. Therefore we expect to see two co-propagating modes at the edge of the material, and one counter-propagating mode, leading to a net chiral current.

It is interesting to note from Fig.[2], that a topological phase transition can be induced by varying the orientation of the in-plane magnetic field. It is also worth noting that at $\Delta = 0$, and at zero temperature, the system is a quantum anomalous Hall insulator for *any* magnetic field strength.

The primary result of the current work is Fig.[2], relevant for buckled lattices. Specifically, that chiral edge states can be created, akin to Haldane's model introduced in 1988, for buckled lattices in an in-plane magnetic field. I now turn my attention to the inclusion of spin, and some notes on possible experimental realizations of this novel result.

So far I have completely neglected spin. The Chern numbers reported in the phase diagram Fig.[2] for a fermionic system are *per spin*. For spin degenerate systems such as that considered here, each spin species will co-propagate. The Zeeman splitting will not affect the Chern number, but if it is larger than the flux gap it will move the bulk bands of one spin species across the Fermi energy. Experimentally, this is an added complication, and will be addressed briefly toward the end of the paper. Therefore, rather than having a total Chern number in Hamiltonian Eq. [1] of 1, for a spinful fermionic system, there is an extra factor of 2 for the spin degeneracy, and the Chern number is in fact 2, corresponding to a $\nu = 2$ quantum Hall effect, with 2 filled Landau levels.

In order to produce a spinful fermionic system with a total Chern number of 1, spin orbit coupling is required. Here we add a spin index to Eq. [1], and introduce the Kane-Mele spin orbit coupling term between next nearest neighbors [2]:

$$H_{SO} = \frac{\lambda_{SO}}{3\sqrt{3}}\sum_{\langle\langle i,j\rangle\rangle,\sigma,\sigma'}\nu_{ij}c^\dagger_{i\sigma}\sigma^z_{\sigma\sigma'}c_{j,\sigma'}, \qquad (7)$$

where $\nu_{ij} = \pm 1$ depending on whether a left or right turn was required in order to hop between the two sites via nearest neighbor bonds. In silicene, $\lambda_{SO} \approx 4$ meV[11]. The low energy expansion of such a term acts as a mass with different signs in all of the sublattice, valley, and spin degrees of freedom. Therefore it modifies the gap $\Delta_{K_\pm}$ such that [13] $\Delta_{K_\pm,s} = \Delta \pm \Delta_\phi \pm s\lambda_{SO}$, where $s = \pm$ corresponds to spin. When $\lambda_{SO} + \Delta > \Delta_\phi$, a mass inversion occurs *for a single spin species, in a single valley* in the Brillouin zone. This in turn leads to

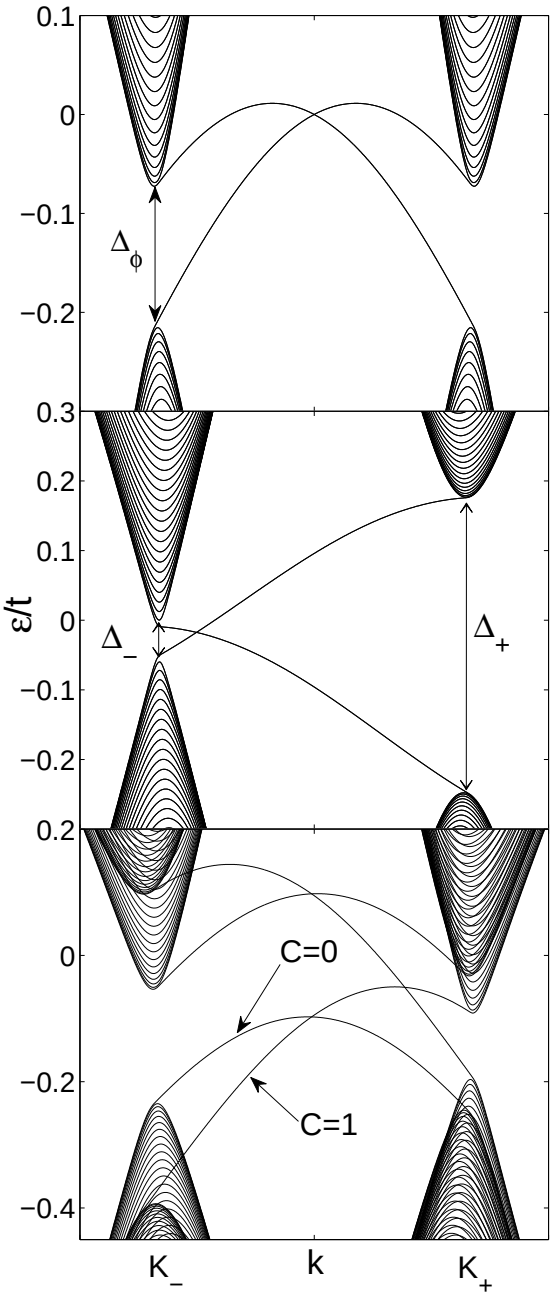

FIG. 4: Dispersion of energy eigenstates for ribbons of: Silicene at $\lambda_{SO} = 0$ (upper), and $\Delta = 0$, the Haldane model (middle) with $\Delta = 0.05t$, and silicene with $\lambda_{SO} = 0.07t$, $\Delta = 0.05t$ (lower). While the Haldane model has a single chiral mode per edge, silicene without spin orbit coupling has three modes per edge, per spin, one of which is counter-propagating with respect to the other two (and one of which cannot be seen as it is too close to the bulk bands). Therefore the Chern number in the two systems (per spin) is the same. In order to obtain a Chern number of 1 in a spinful system, spin orbit coupling must be introduced. In the lower pane, λ_{SO} has caused a band inversion for one K-point, and one pseudo-spin, such that this band becomes topologically trivial, while the other pseudo-spin retains a Chern number of 1. The other parameters for the silicene systems: $t' = 0.1t$, $\phi/\phi_0 = \pi/2$, and $\theta = \pi/2$.

the destruction of a single edge state, and thus a total Chern number of 1. From the phase diagram Fig.[2], the way to understand this is that one species has mass $\Delta_\phi > \Delta - \lambda_{SO}$, and thus $C_n = 1$, whereas the other has $\Delta_\phi < \Delta + \lambda_{SO}$, and thus $C_{tot} = 1$. For larger spin orbit couplings however, a second mass inversion takes place, when $|\Delta - \lambda_{SO}| > \Delta_\phi$, such that the system becomes equivalent to the original quantum spin Hall insulator [2], with counter-propagating edge states. These phases are all indicated in the spinful phase diagram, Fig.[3].

In Fig.[4], zig-zag edged ribbons of silicene with and without spin orbit coupling, together with the Haldane model are shown. For spin degenerate silicene (i.e. neglecting Zeeman splitting), we see that there is a single band (per edge) with three propagation directions, or two turning points, per band. These three propagation directions correspond to the three cyclotron orbits discussed earlier in the context of Fig.[1]. For the sake of comparison, the Haldane model is also shown in the middle pane, which just has a single propagation direction per edge. These two figures emphasise the contrast of the mechanisms of the Haldane and silicene models.

The lower panel in Fig.[4] shows the effect of the spin orbit coupling on the edge states. As discussed, the spin orbit interaction inverts the mass of a single spin species at a single valley, thus producing a single anticrossing in comparison with the spin degenerate case. This in turn leads to a Chern number of 0 for one edge state, and a Chern number of 1 for the other.

Finally, I estimate the magnetic field needed to produce a Haldane-like model in a real system. For any finite magnetic field, at zero temperature, silicene is a Chern insulator. However, in order to obtain a chiral edge state per spin, an appreciable flux gap must be formed by the magnetic field in order to obtain edge states not lost to thermal fluctuations. For silicene, the next nearest neighbor bonds are separated by $\approx 4\,\mathring{A}$, and the vertical buckling amount is $\approx 0.46\,\mathring{A}$. Therefore $\phi/\phi_0 \approx 2\times10^{-5}\,\mathrm{T}^{-1}$. Unfortunately, for small fields, the flux-gap Eq. [4] goes as ϕ^3, as mentioned earlier, and so an extremely large field (~ 100 T) is required to obtain a gap of only $2\mu K$. This is clearly unrealistic.

A more feasible scenario can be obtained by inducing next nearest neighbor hopping anisotropy. As alluded to earlier, this can be achieved by the inclusion of a plane polarized laser. This can be understood as the hopping parameters being adjusted, in the same manner as by the Peierl's substitution, by a time averaged gauge field. More concretely, in the regime $\hbar\omega \ll \Delta_{K_-}$, this modifies the hopping matrix elements such that $t \to J_0(eaE/\hbar\omega)t$ by Floquet theory [14, 15], where $\vec{E} = E_0\cos(\omega t)\hat{E}$, and a is the lattice constant. As an example, this modifies the gap equation Eq. [4] such that, for an electric field polarized in the plane parallel to $\theta = 0$, and for small ϕ

$$\Delta_\phi = \sqrt{3}t'\phi/\phi_0|(J_0(eaE_0/2\hbar\omega) - J_0(eaE_0/\hbar\omega))\sin(3\theta)|, \quad (8)$$

where J_0 is the modified Bessel function of the second kind. For a low frequency, high intensity laser, the flux gap will increase linearly, and appreciably, with ϕ. It is clear then that if the next nearest neighbor hopping can be modified such that the Bessel function difference in Eq. [8] is optimised, a measurable flux gap may become feasible. As a concrete example, for a 2.5 THz laser, where $\hbar\omega = 10$meV, at an intensity of 5×10^7 Vm^{-1}, a flux gap of $\Delta_\phi \approx 1.3t'\phi/\phi_0$ is achievable, which, for a 35 T field, is ≈ 0.5 K.

Another route to realising anisotropic next nearest neighbor hopping is via uni-axial strain. In this case, the flux gap is modified as $\Delta_\phi \propto \delta t'\phi$, where $t' \to t' + \delta t'$ along the strain axis. However, the added complication of emergent gauge fields must be taken into account in this case [16].

In both of the above examples, the Zeeman splitting will likely cause bulk bands for one K point to cross the Fermi surface. For a g-factor of 2, the Zeeman splitting at 35 T is $\sim$ 20 K, which in the specific example mentioned above, is much larger than the flux gap. I emphasise however, that the Zeeman splitting does not affect the Chern number in any way. Away from the K points, the bulk bands will still be gapped in general, and so the gapless edge states could feasibly be imaged with angle resolved photoemission spectra. Alternatively, the edge states could be measured via a nonlocal transport experiment, using an H-bar type geometry, which is precisely the way in which 2D topological insulator edge states have been compellingly verified [18]. In order to obtain a bulk gap however, the Zeeman splitting must be less than the flux gap, and so the plaquette area must be maximized and/or the next nearest neighbor hopping must be large, or a material used where the g-factor is suppressed.

More exotic systems may be employed to maximize the staggered flux through the unit cell. For instance, bilayer systems can be envisaged where the inter-layer gap becomes much larger than that reported here, due to the vastly increased interlayer spacing. Another possibility is that the "designer Dirac fermions" engineered by precise placement of carbon monoxide molecules to produce "molecular graphene" [17] could be engineered to produce a buckled structure with large out-of-plane displacement, and/or strong next nearest neighbor coupling and anisotropy.

In conclusion, I have introduced a new conceptual framework whereby Haldane-like models can be realised. The key material property in this proposal is a buckled lattice, such that an in-plane magnetic field produces a unit cell with zero net flux, yet regions with positive and negative flux which individually support cyclotron orbits. In this way, the chirality necessary in implementing a Haldane-like model can be realised. Using silicene as a specific example, I showed that over a range of field angles, silicene in an in-plane field is topologically equivalent to the Haldane model per spin, with chiral edge states arising by similar, yet distinct physical processes, and that topological phase transitions can be induced by rotating the orientation of the field. The physical realization of a Haldane-like model in a condensed matter system would be a remarkable achievement.

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